AN ATTEMPT OF STRUCTURE REFINEMENT OF QUARTZ. By K. Akaogi, Depto. Fisica, USP, Sio Carlos, SP, Brazil; Y. Yumura and T. M. Akaogi, Inst. Fis., UFRJ, Rio de Janeiro, RJ, Brazil; and Y. P. Masecasto, Inst. Fis., Quim., São Carlos, USF, São Carlos, SP, Brazil.

The synthetic compound Fe\textsuperscript{3+}Fe\textsuperscript{2+}(PO\textsubscript{4})\textsubscript{2}(OH\textsubscript{2})\textsubscript{n} is tetragonal, space group P4\textsubscript{2}12\textsubscript{1}, c = 7.310(3) \AA, Z = 4, D = 3.084(1) g.cm\textsuperscript{-3}, u = 63.1 cm\textsuperscript{-1}. The structure was solved by the heavy atom technique and refined by the least-squares method to an R value of 0.108 for 347 observed reflections. The structure consists of two disordered Fe\textsuperscript{3+} ions in special positions and one Fe\textsuperscript{2+} ion in general position, octahedrally coordinated by (PO\textsubscript{4})\textsuperscript{3-} ligands and (OH\textsubscript{2})\textsuperscript{-} groups. The octahedra form infinite face sharing chains alternatively in the [1 1 0] and [1 \bar{T} 0] directions. Unusual features of the structure include a Fe\textsuperscript{3+}-OH distance of 2.26 Å and a mean-value of 0-O'/edges of 2.74 Å of octahedral shared faces.

This work has received the support of FINEP, CNPq, FAPESP and CAPES which are hereby gratefully acknowledged.

THE CRYSTAL STRUCTURE OF SYNTHETIC LIPSCOMBITE: A REDETERMINATION. By J. L. Wang, Department of Chemistry, University of Virginia; T. C. Hawthorne, Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2; B. L. Sherriff, Department of Geology, McMaster University, Hamilton, Ontario, L8S 4H4; J. S. Hartman, Department of Chemistry, Brock University, St. Catharines, Ontario, L2S 3A1.

We have used single-crystal structure refinement, IR and MAS NMR spectroscopies to investigate OH=F substitution in the amblygonite- montebasite series. 

OH=F SUBSTITUTION IN THE AMBLYGONITE-MONTEBASITE SERIES: A CRYSTAL STRUCTURE AND SPECTROSCOPIC STUDY. By J. A. Groat, M. Rausch, F. C. Hawthorne, Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2; B. L. Sherriff, Department of Geology, McMaster University, Hamilton, Ontario, L8S 4H4; J. S. Hartman, Department of Chemistry, Brock University, St. Catharines, Ontario, L2S 3A1.

The infrared spectrum of the near OH end member showed a sharp peak at 3390 cm\textsuperscript{-1}, corresponding to the principal (0-H) stretching band. With progressive F=OH substitution, this peak rapidly broadened and shifted to lower wave-numbers, reaching 3355 cm\textsuperscript{-1} for F/(OH)=0.70. All samples had a reasonably smooth envelope in this region, except for the 0.70 F/(OH)= sample, which had a distinct shoulder on the high energy side of this band. The 27Al MAS NMR spectra gave a broad peak at ~157 ppm that was insensitive to F/(OH) ratio. The 27Al spectrum gave a broad peak that decreased in width and shifted to slightly lower field with increasing F content. A TEM study is in progress to investigate the possibility of a variable domain structure across the series.